

IV.C.9 Advanced Water-Gas-Shift Membrane Reactor

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Objectives

- Identify a suitable Pd-Cu tri-metallic alloy membrane with high stability and commercially relevant hydrogen permeation in the presence of carbon monoxide and trace amounts of sulfur.
- Identify and synthesize a water-gas-shift (WGS) catalyst with a high operating life that is sulfur and chlorine tolerant at low concentrations of these impurities.

Technical Barriers

This project addresses the following technical barriers from the Separations and Other Cross-Cutting Hydrogen Production section (3.1.4.2.3) of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- L. Durability
- M. Impurities
- N. Defects
- O. Selectivity
- P. Operating Temperature
- Q. Flux
- S. Cost

The project also addresses one or more of the barriers described in Section 5.1.5.1., Technical Barriers – Central Production Pathway in the Hydrogen from Coal – Research, Development, and Demonstration Plan, which was issued by the DOE Office of Fossil Energy.

Technical Targets

This project is conducting atomistic and thermodynamic modeling studies to identify a Pd-Cu tri-metallic alloy membrane with high stability to provide commercially-relevant hydrogen permeation rates in the presence of trace amounts of carbon monoxide and sulfur. The project effort will also seek to identify and synthesize

a WGS catalyst with a high engineering and operating lifetime, which will also be sulfur and chlorine tolerant at low concentrations of these impurities.

Tables 1 and 2 list the targets that the project will attempt to meet during its implementation.

Table 1. Technical Targets: Ion Transfer Membranes for Hydrogen Separation and Purification^a

Performance Criteria	Units	2003 Status	2005 Target	2010 Target	2015 Target
Flux Rate	scfh/ft ²	60	100	200	300 ^b
Cost	\$/ ft ²	2,000	1,500	1,000	<\$500
Durability	Hours	<8,760	8,760	26,280	>43,800
ΔP Operating Capability	psi	100	200	400	400-1000
Hydrogen Recovery	% of total gas	60	>70	>80	>90
Hydrogen Purity	% of total (dry) gas	>99.9	>99.9	>99.95	99.99

^a Targets are derived from Table 3.1.5. from the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan, March 2005.

^b Flux upper limit for ion transport membranes.

Table 2. Technical Targets for the Water Gas Shift Reaction^c

Performance Criteria	Units	Current Status	2005 Target	2010 Target	2015 Target
Reactor Type	–	Multiple Fixed beds		To be determined	
Catalyst Form	–	Pellets		To be determined	
Active Metal	–	Cu/Zn or Fe/Cr or Co/Mo		To be determined	
Temperature	°C	200-550	300-450	300-500	200-600
Pressure	psia	450-1150	450	750	>1,000
Approach to Equilibrium	°C	8-10	10	6	<4
Min Steam/Co Ratio	Molar	2.6	3.0	2.5	<2
Sulfur Tolerance	–	Varies	Low	Moderate	High
Chloride Tolerance	–	Varies	Low	Moderate	High
Water Tolerance	–	Varies	Low	Moderate	High
Stability/Durability	Years	3-7	3	7	>10
Reactor Cost Reduction	%	–	–	>15%	>30%

^c Targets are derived from Table 6 of the Hydrogen from Coal RD&D Program, June 10, 2004.

Approach

- Identify, through a combination of atomistic and thermodynamic modeling, a suitable Pd-Cu tri-metallic alloy membrane that displays high stability and produces a commercially relevant hydrogen permeation rate of under 42 atm of H₂, CO, CO₂, and H₂O containing ~8.8 atm partial pressure of carbon monoxide and 0.004 atm partial pressure H₂S (~100 ppm) in the presence of at least 24 atm of steam.
- Identify and develop a WGS catalyst with robust qualities and high operating life-time through a combination of atomistic modeling to identify target catalyst structures, catalyst synthesis to realize these

structures, micro-reactor kinetics determination, and > 1000 hour life testing. The target catalyst activity is a projected precious metal turnover frequency of 0.5 moles CO/moles total precious metal/sec at ~400 °C after 45,000 hours of operation under 42 atm of cleaned, oxygen-blown coal gas with a H₂O/CO ratio of ~3 and containing about ~100 ppm sulfur species.

Accomplishments

This project is newly initiated and no there are no accomplishments to report to date.